



**PDC Center for  
High Performance Computing**



**National Supercomputer Centre  
at Linköping University**

# NSC & PDC

## Resource and Technology Providers for SeRC

Erwin Laure  
Director PDC-HPC

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Director NSC

# NSC & PDC



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- Two leading Swedish HPC centers within the Swedish National Infrastructure for Computing (SNIC)
- Founded in 1989 (NSC) and 1990 (PDC)

# Resources and Technologies for eScience



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- eScience is critically dependent on the provision of excellent resource for
  - Networking (by SUNET)
  - Computing (by NSC & PDC)
  - Storage (by NSC & PDC)
  - Visualization (by LiU and KTH)
- To make efficient use of these resource expert support and advanced technologies are needed
  - Advanced algorithms
  - Parallelization
  - Distributed computing
  - Data storage and management
  - Task of “core eScience” together with NSC & PDC

# NSC & PDC inside SeRC



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- Major resource and technology providers
- Swedish bridgehead for European e-Infrastructures (EGI, PRACE)
- Thanks to SeRC NSC and PDC are in the process of better aligning their strategies and support
  - Complementary competences
  - Harmonized user environment
  - Joint application support on major systems
  - MoU signed by KTH and LiU rektors





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# Systems



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# SNIC Resources at PDC

- **Ekman**

KAW-funded system for Climate and Flow research  
10,144 cores (1268 nodes, 2 quad core AMD)  
89 TF theoretical peak performance  
20 TByte memory

- **Ferlin**

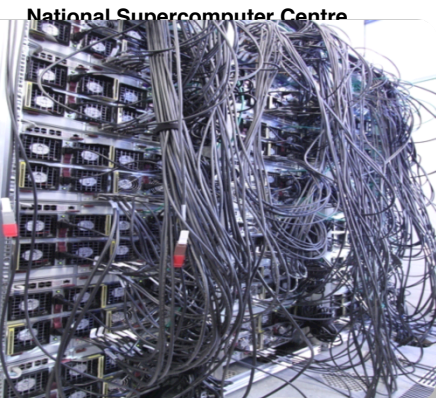
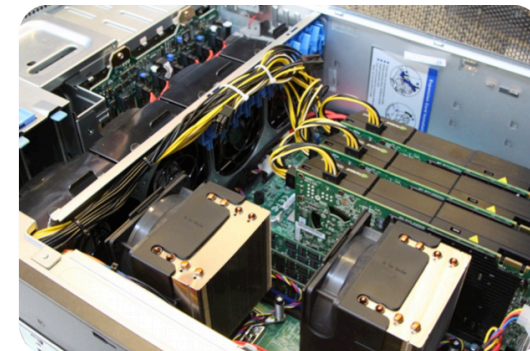
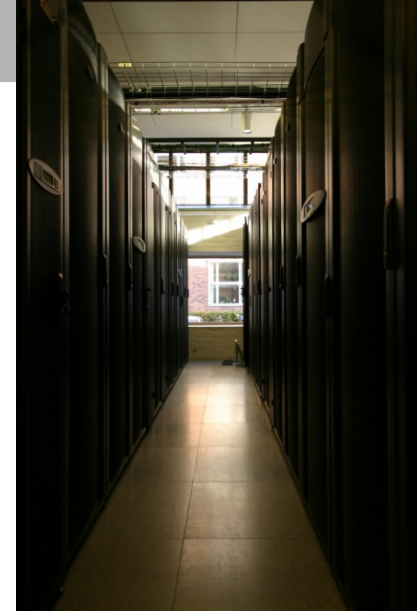
SNIC Throughput System  
6,120 cores (765 nodes, 2 quad core Intel)  
7 TByte memory  
Will be decommissioned end of 2011 – application  
for replacement system filed with SNIC

- **Zorn**

GPU cluster for VIC-Stockholm  
14 GPUs, 14 TF SP, 6.25 TF DP  
Currently being upgraded to 38 GPUs thanks  
to SNIC co-funding

- **Povel**

Prototype system for PRACE  
4320 cores (180 4x6core AMD nodes)  
36 TF theoretical peak performance  
5.76 TByte memory



# Lindgren – SNIC's PRACE Tier-1 System



- Cray XE6
- 2 12core AMD Opteron CPUs 2.1 GHz, 32 GB RAM per node
- 1516 compute nodes (36,384 cores), 305 TF TPP, 237 TF sustained
- Gemini 3D torus network
- Nr. 9 in Europe and Nr. 31 worldwide on the June 2011 Top500 list





# Major HPC systems at NSC



- **Neolith**

- SNIC Capability cluster
- 805 nodes (6440 cores), 60 TF TPP
- HP ProLiant DL140 G3 with 2 Quad-Core Intel Xeon processors, 2.33 GHz, 16--32GB RAM
- Cisco DDR Infiniband, Full bisection bandwidth
- Total 14 TiB RAM
- 23rd rank on TOP-500 list when delivered

- **Kappa**

- SNIC Capacity cluster
- 364 nodes (2912 cores), 26 TF peak, 12 TiB RAM
- HP ProLiant DL170h with 2 Quad-Core Intel Xeon E5520, 2.26 GHz, 24--72 GB RAM (72 nodes with 72 GB)
- Voltaire QDR Infiniband

- **Matter**

- KAW-funded system for material sciences (LiU, KTH, UU)
- 516 nodes (4128 cores), 37 TF TPP, 19 TiB RAM
- HP ProLiant SL2x170z with 2 Quad-Core Intel Xeon E5520, 2.26 GHz, 36--144 GB RAM
- Voltaire QDR Infiniband



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# Triolith

– next capability system at NSC



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- **Triolith currently procured, in service by end of 2012**
  - SNIC Capability cluster
  - 1200 nodes (19200 cores), **338 TF TPP**
  - HP ProLiant SL6500 Scalable System, SL230s Gen8 nodes with Intel E5-2660 2.2GHz  
8 cores, Mellanox FDR 2:1, 32–128 GB RAM
- **Additional systems for SMHI and Saab**

# Additional HPC systems at NSC

- **Byvind**

- System for weather forecasts (SMHI)
- 140 nodes (1120 cores), 12 TF TPP, 3.3. TiB RAM
- HP ProLiant SL2x170z with 2 quad-core Intel Xeon X5550, 2.66 GHz, 24 GB RAM

- **Bore/Gimle**

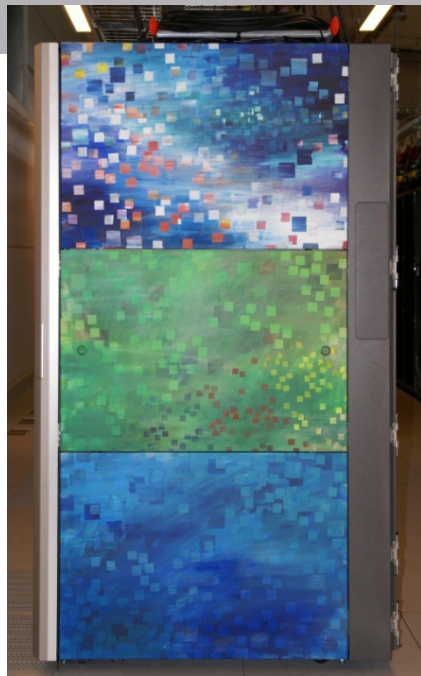
- System for weather forecasts and climate calculations (SMHI)
- 268 nodes (2144 cores), 22 TF TPP, 5.3 TiB RAM
- 140 HP ProLiant DL160 with 2 QuadCore Intel Xeon E5462, 2,8 GHz, 16 GB RAM
- 128 HP ProLiant DL170h with 2 QuadCore Intel Xeon E5520, 2,26 GHz, 24 GB RAM
- Cisco DDR and Voltaire DDR Infiniband

- **Skylord**

- System for calculations at Saab
- 108 nodes (456 cores), 5,4 TF peak, 776 GiB RAM
- 40 HP ProLiant DL160 with 2 QuadCore Intel Xeon E5462, 2.8 GHz, 16 GB RAM
- 68 ACT Supermicro with 2 Intel Xeon, 3,4 GHz, 2 GB RAM
- Cisco DDR Infiniband and Gigabit

- **Smokerings**

- SNIC Swegrid system
- 66 nodes (448 cores) , 5,6 TF peak, 1 TiB ram
- ACT Supermicro with 2 QuadCore Intel Xeon E5430, 2,66 GHz, 16 GB RAM
- HP Gigabit network



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# Storage



- $\sim 5.4$  PB disk @ NSC
  - NSC centre-common storage and SMHI storage
  - Posix file system (mounted as NFS, GPFS or Lustre)
- 500 TB DDN Lustre storage at PDC
  - Evolves into site-wide storage
- AFS-based home directories
  
- IBM tape robots both at NSC and PDC ( $\sim 2900$  slots,  $\sim 3.0$  PB)
  - Accessible via HSM, TSM, dCache, and MARS
  
- Large users
  - WLCG (high-energy physics at CERN)
  - IceCube (neutrino observatory at the South Pole)
  - BILS/ELIXIR (Bioinformatics infrastructures)
  - ECDS (Environment Climate Data Sweden)
  - INCF (Allan Brain Atlas, Waxholm Space ...)
  - ODIN Space Mission
  - Human Proteome Project
  
- Swestore national storage



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**Integrated Capacity of > 1 PFs**



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# Issues



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- Lack of capacity resources (throughput oriented resources) within SNIC
  - Will get worse with Ferlin retiring
  - NSC and PDC have filed applications but no decision so far
- Despite recent investments in capability resources (Abisko @ HPC2N, Triolith @ NSC) we will soon see shortage of capability resources as well
  - Particularly when Ekman retires
  - PDC and NSC will make a joint case to SNIC

# PDC is going green: Heat Reuse Project



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- Background: today around 1.3 MW used at PDC
- Project started 2009 to re-use this energy
- Goals:
  - Save cooling water for PDC
  - Save heating costs for KTH
  - Save the environment
- Use district cooling pipes for heating when no cooling is required
- No heat pumps
- Starting with Cray
- First phase of Cray will heat the KTH Chemistry building





# Application Support



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- NSC and PDC provide advanced application support
  - Installation and tuning of application software
  - Advice on efficient resource usage
  - Hardware selection
  - Performance tuning and code optimization



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# Application expertise



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- Domain-specific
  - Bioinformatics
    - Joel Hedlund (NSC)*
    - NN (NSC)*
    - NN (PDC)*
  - Comp. Chemistry
    - Torben Rasmussen (NSC)*
    - Olav Vahtras (PDC)*
  - Materials sciences
    - Peter Larsson (NSC)*
    - Weine Olovsson (NSC)*
  - Climate
    - Chandan Basu (NSC)*
    - NN (NSC)*
  - Neuroinformatics
    - Mikael Djurfeldt (PDC)*
  - Molecular Dynamics
    - Rossen Apostolov (PDC)*
  - CFD
    - Jing Gong (PDC)*
- E-science coordination
  - Johan Raber (NSC)*
- Code optimisation
  - Chandan Basu (NSC)*
  - Soon-Heum Ku (Jeff, NSC)*
  - Yuanyuan Zhang (NSC)*
  - NN (NSC)*
  - Jonathan Vincent (PDC)*
- Software development
  - Krishnaveni Chitrapu (NSC)*
  - Andreas Lindqvist (NSC)*
  - Per Lundqvist (NSC)*
- PRACE
  - Lilit Axner (PDC)*
- Clouds
  - Zeeshan Ali Shah (PDC)*

# Open Vacancies



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## Application experts

- Bioinformatics at PDC
- Bioinformatics at NSC
- Neuroinformatics at PDC
- Climate at NSC

## System Expert

- Earth System Grid Climate Data at NSC

# Selected New Activities



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- Cloud testbed @ PDC
  - Develop and test cloud services
  - Started with complex disease community
- VIC GPU testbed @ PDC
  - Operated for VIC-Stockholm
  - Now a national pilot together with NSC that hosts an experimental system with new hardware
- Exascale Research @ PDC
  - EC Project "CRESTA" started in autumn 2011
    - Peta- and Exascalng of selected codes:
    - GROMACS, NEK5000 @ KTH
    - OPENFOAM @ Stuttgart
    - ELMFIRE @ CSC
    - IFS @ ECMWF
    - HemeLB @ UCL
- NSC Express
  - User-friendly self-service interface for NSC users
- SUPR – SNIC User and Project Repository
  - New SNAC application system
  - Created by NSC in collaboration with C3SE
- Setting up ESG data node for SMHI/IS-ENES @ NSC

# International Dimension



- Swedish bridgehead for European e-Infrastructures
  - Provide resources to European e-Infrastructures under the coordination of SNIC
  - Support Swedish users in gaining access to them

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[www.swegrid.se](http://www.swegrid.se)  
SweGrid





## PRACE open calls

There are three types of call:

- **Tier-0** call for applications – open every 6 months

To get only **CPU time** on one of the PRACE six **Tier-0** systems

- **DECI (Tier-1)** call for applications – open every 6 months

To get both **CPU time and expert help** up to 6 months on one of the many **Tier-1**

systems across PRACE partners.

- Preparatory access calls – **constantly open**

We encourage you to apply for the preparatory access calls to get an **expert help** for 6 months to scale your code on **Tier-0** systems

## Tier-0 accepted applications

So far only one Swedish application has been accepted for Tier-0 call

**REFIT - Rotation effects on flow instabilities and turbulence**

**Project leader:** Arne Johansson, KTH Department of Mechanics, Sweden

**Computer system:** JUGENE, GAUSS/FZJ

**Resource awarded:** 46 000 000 core-hours (Nov 2011-Oct 2012)

## DECI7 (Tier-1) call: November 2011 – November 2012)

**DECI7 – 35 EU projects have been accepted out of which 4 are Swedish**

- 1. Project Name:** DiSMuN (Diffusion and spectroscopical properties of multicomponent nitrides)  
**Principal Investigator:** Prof. Igor Abrikosov  
**Research area:** Materials science
- 2. Project Name:** SPIESM (SPIESM : Seasonal prediction improvement with an Earth System Model)  
**Principal Investigators:** Dr Colin Johns and Prof. Francisco Doblas-Reyes  
**Research field:** Earth Sciences and Environment
- 3. Project Name:** MUSIC  
**Principal Investigator:** Dr. Mikael Djurfeldt  
**Research field:** Computational Neuroscience
- 4. Project Name:** SIVE-2  
**Principal Investigator:** Prof. Erik Lindahl  
**Research area:** Biosciences: molecular dynamics simulation of viral entry

## DECI8 (Tier-1) call: May 2012 – May 2013

**DECI8– 33 EU projects have been accepted out of which 4 are Swedish**

- 1. Project Name:** PIPETURB (Large scale simulation of turbulent pipe flow )  
**Principal Investigator:** Dr. Philipp Schlatter  
**Research area:** Engineering, Fluid Dynamics
- 2. Project Name:** PLANETESIM (Towards an initial mass function of planetesimals )  
**Principal Investigator:** Dr. Anders Johansen  
**Research field:** Astro Science
- 3. Project Name:** CANONS (Comprehensive Ab initio studies of Nitride and Oxide fuels and Nuclear Structural materials)  
**Principal Investigator:** Dr. Pär Olsson  
**Research field:** Materials Science
- 4. Project Name:** MBIOMARK (Multifunctional biomarkers for electron paramagnetic resonance imaging)  
**Principal Investigator:** Dr. Zilvinas Rinkevicius  
**Research area:** Materials Science

## DECI9 (Tier-1) call: November 2013 – November 2014

DECI 9 call for applications is open from **April 17th to May 30th**

More information and application form can be found at:

<http://www.prace-ri.eu/Call-Announcements>

Experts that can help you with the application form:

PDC - Lilit Axner lilit(at)kth.se

NSC - Chandan Basu cbasu(at)nsc.liu.se, Soon-Heum "Jeff" Ko sko(at)nsc.liu.se

HPC2N - Mikael Rännar mr(at)cs.umu.se, Jerry Eriksson jerry(at)cs.umu.se

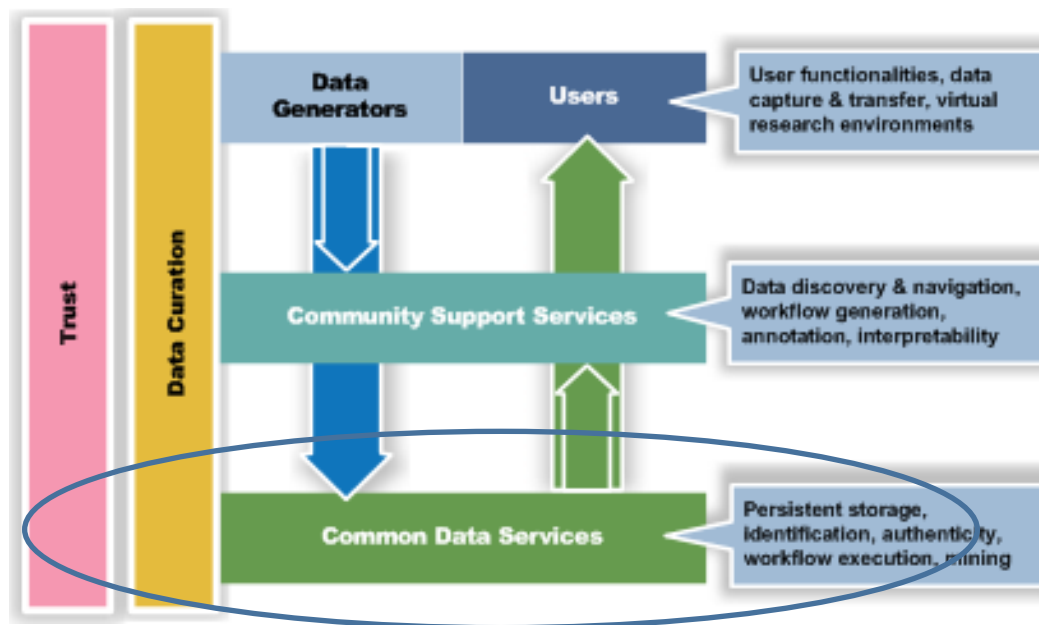
UPPMAX - Biplab Sanyal biplab.sanyal(at)fysik.uu.se, Elias Rudberg elias.rudberg(at)it.uu.se

LUNARC - Joachim Hein joachim.hein(at)math.lu.se

C3SE – Luis Fazendeiro luis.fazendeiro(at)chalmers.se

**Please apply!**

# The Collaborative Data Infrastructure (CDI) concept



# EUDAT Core Service Areas

## Community-oriented services

- Simple Data Access and upload
- Long term preservation
- Shared workspaces
- Execution and workflow (data mining, etc.)
- Joint metadata and data visibility

## Enabling services (making use of existing services where possible)

- Persistent identifier service (EPIC, DataCite)
- Federated AAI service
- Network Services
- Monitoring and accounting

## Core services are building blocks of EUDAT's Common Data Infrastructure

mainly included on bottom layer of data services





# SweStore – national storage



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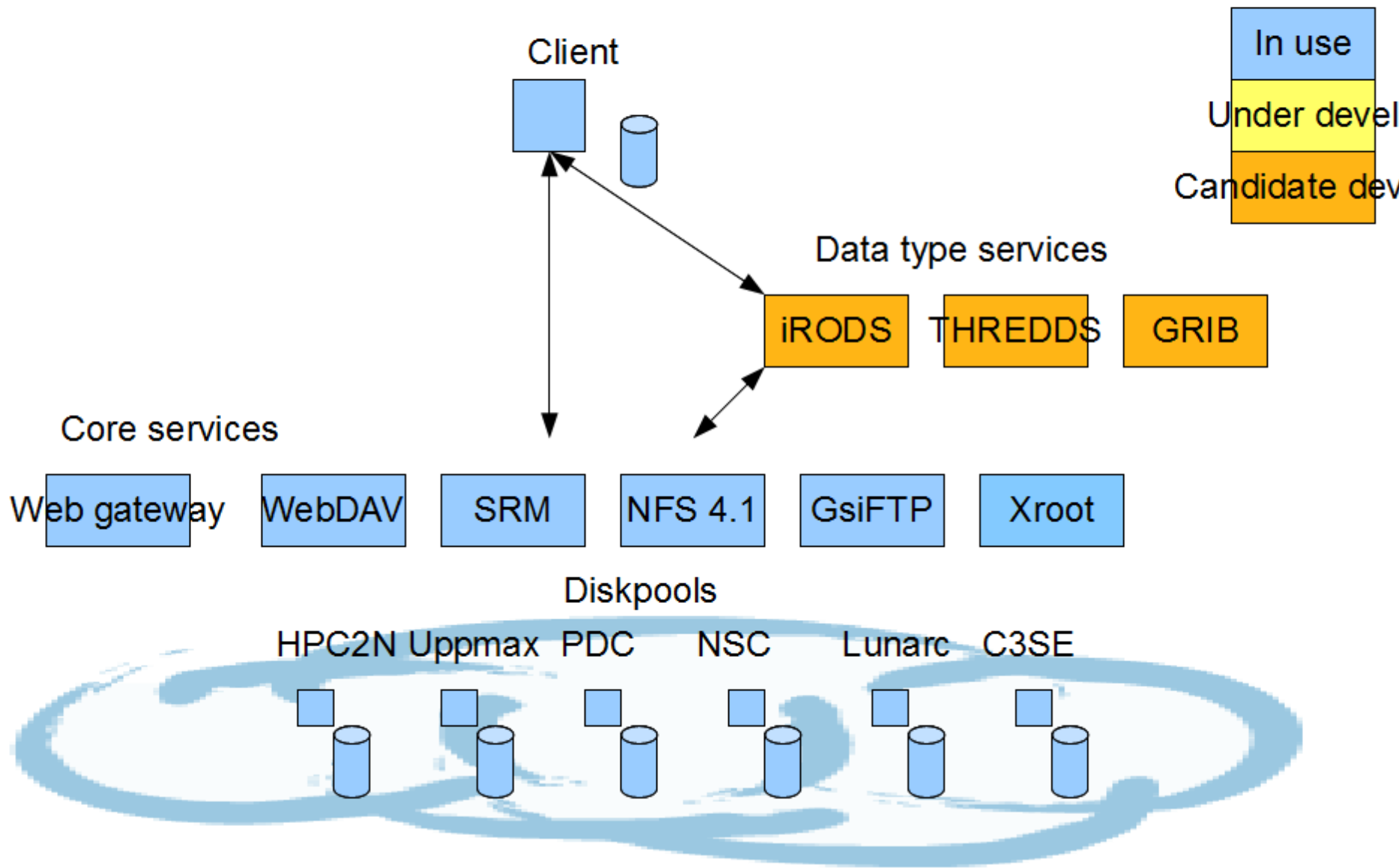


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- Storage system with currently 1200TiB
- One single storage space located at the six SNIC centres
- Based on dCache software
- Collaboration with NorStore, Nordunet, NeIC ....
- Certificate is used instead of regular passwords when accessing the storage system. X.509 certificates uses for identification and authentication purposes



# Access protocol



# To start using Swestore



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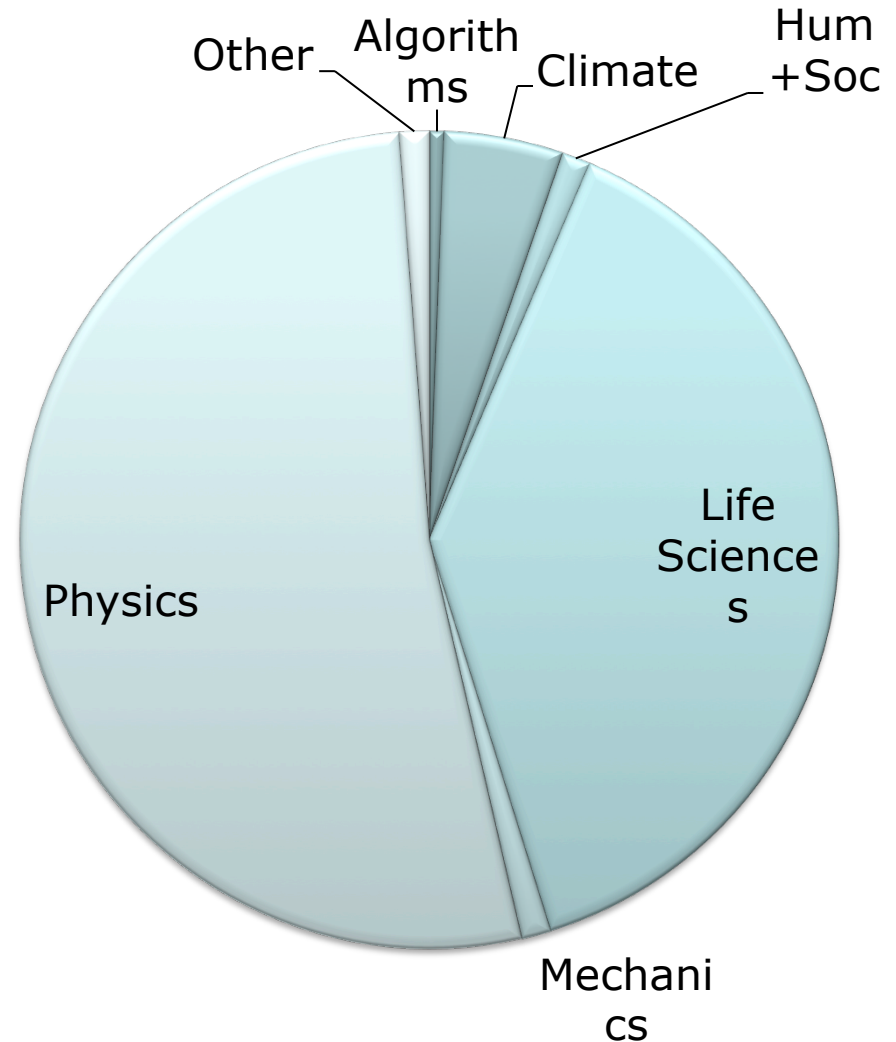
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- Install grid access software
- Get a grid certificate
- Apply for VO and group membership

Find the details at  
<http://snicdocs.nsc.liu.se/wiki/Swestore>

# Swestore usage

Project	TB	Doman
alice	400	Particle physics
amplicons	10	Life sciences
ardnas	5	Life sciences
atlas		Particle physics
baltic_abyss	10	Life sciences
bbmri	10	Life sciences
bils	10	Life sciences
biogrid	10	Life sciences
brain_protein_atlas	10	Life sciences
cesm1_holocene	30	Cimate
congenie	30	Life sciences
Chemo	5	Life sciences
dnsturb	10	Mechanics
eliasrudberg	5	Algorithms
genomics-gu	10	Life sciences
HTP3d	10	Life sciences
icecube	40	Particle physics
IFM-Bioinformatics	3	Life sciences
klasm	10	
linnarsson_mbb	10	Life sciences
snd-hms	10	Hum+Soc sci
snd-km	10	Climate
subatom	10	Physics
uppnex	200	Life sciences
<b>Sum</b>	<b>858</b>	



# Summary



**PDC Center for  
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- NSC and PDC are the major resource and technology providers for SeRC
- Increased collaboration and harmonization thanks to SeRC
- Ensure efficient access to European e-Infrastructures